

Data Path : Z:\HPCHEM1\BNA G\DATA\BG082316\
 Data File : BG023876.D
 Acq On : 24 Aug 2016 5:32
 Operator : UM/SJ
 Sample : H4528-18
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 VITALEFILL-MCMPH3-5

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA G\Methods\8270-BG080116.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.970	16	22	42	rBV	6015366	11867459	100.00%	20.470%
2	5.155	388	394	406	rVB	772311	1199076	10.10%	2.068%
3	5.631	468	475	487	rBV	2045426	3505900	29.54%	6.047%
4	7.252	743	751	763	rBV	2119071	3897857	32.84%	6.723%
5	7.616	805	813	827	rBV	2095402	3800640	32.03%	6.556%
6	8.092	885	894	903	rBV	467260	809010	6.82%	1.395%
7	8.415	940	949	959	rBV	1531916	2706131	22.80%	4.668%
8	9.267	1086	1094	1108	rBV	1303905	2462660	20.75%	4.248%
9	10.924	1368	1376	1385	rBV	607127	1119796	9.44%	1.932%
10	13.373	1784	1793	1804	rBV	3010376	4810443	40.53%	8.298%
11	14.207	1927	1935	1941	rBV	771978	1175112	9.90%	2.027%
12	14.766	2022	2030	2042	rBV2	940404	1536972	12.95%	2.651%
13	15.582	2165	2169	2174	rVB2	90646	122320	1.03%	0.211%
14	16.264	2278	2285	2295	rBV	2615640	4220523	35.56%	7.280%
15	16.451	2312	2317	2324	rBV	113247	189976	1.60%	0.328%
16	17.527	2493	2500	2513	rBV	1266199	1962047	16.53%	3.384%
17	18.396	2643	2648	2658	rBV2	153923	245218	2.07%	0.423%
18	20.135	2938	2944	2951	rBV	5532962	7279119	61.34%	12.556%
19	21.439	3162	3166	3177	rBV5	121612	282651	2.38%	0.488%
20	21.844	3228	3235	3248	rVB	1270883	2288496	19.28%	3.947%
21	23.348	3487	3491	3499	rVB5	63308	125172	1.05%	0.216%
22	24.194	3631	3635	3642	rVB3	65524	134331	1.13%	0.232%
23	25.216	3798	3809	3821	rVB	691891	2233052	18.82%	3.852%

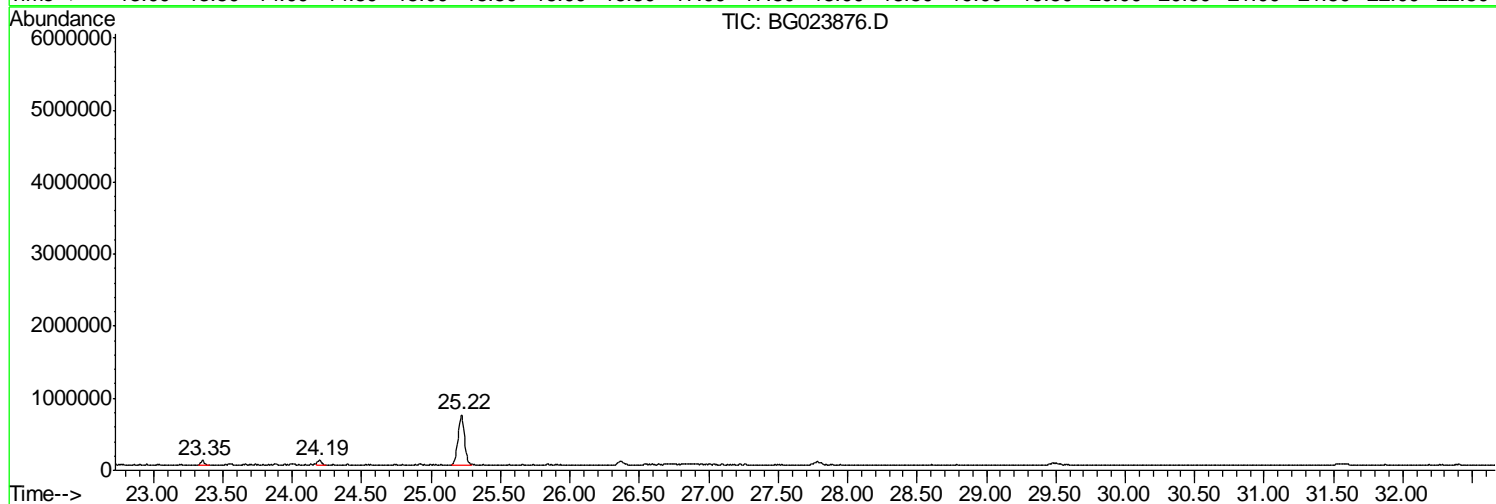
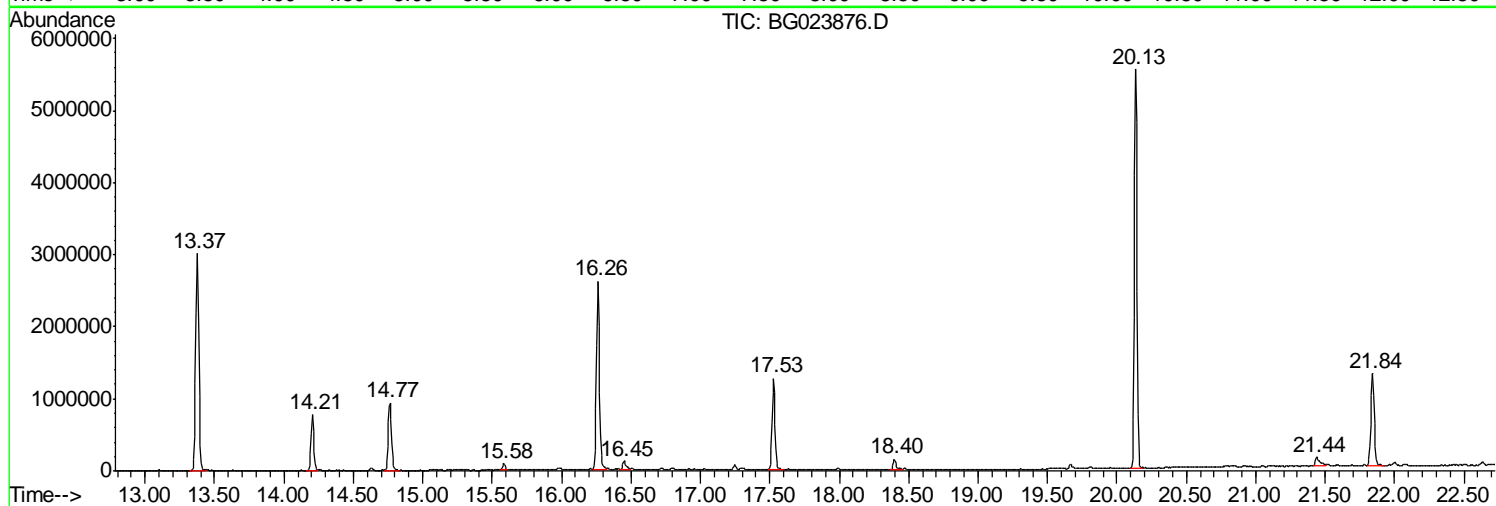
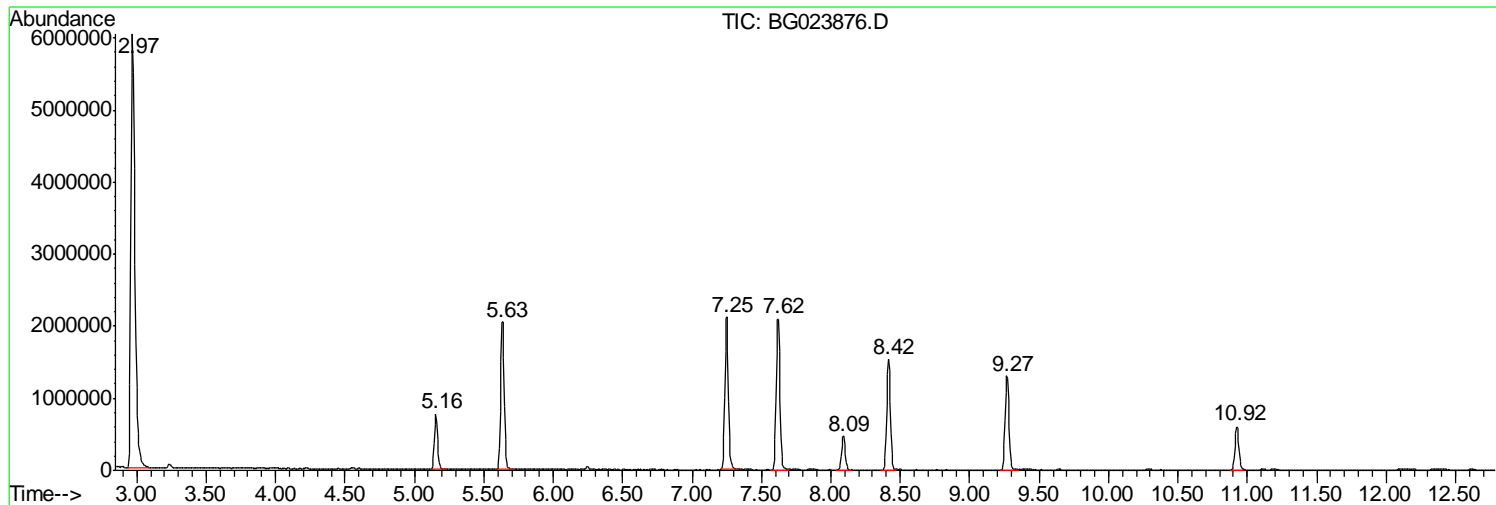
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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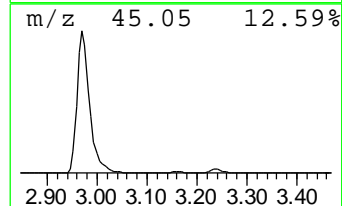
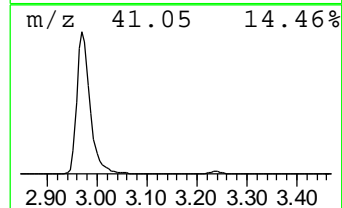
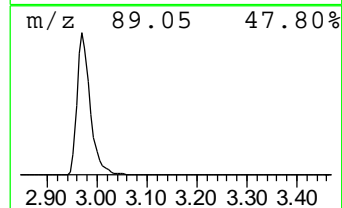
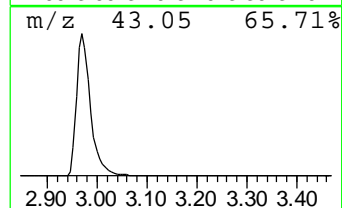
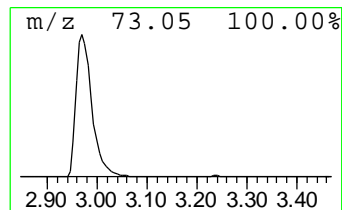
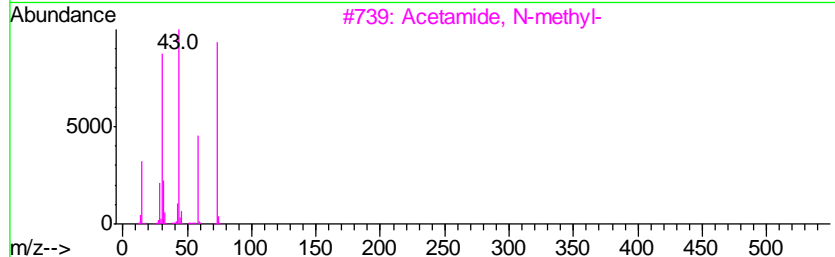
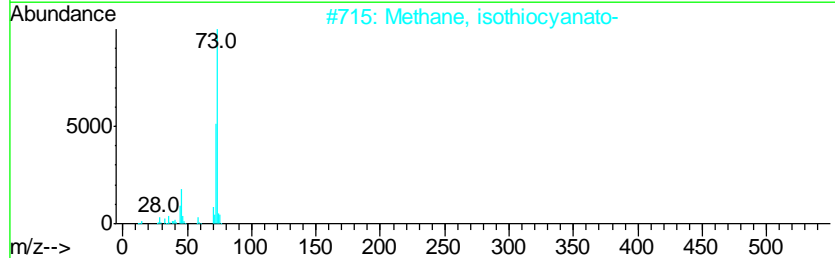
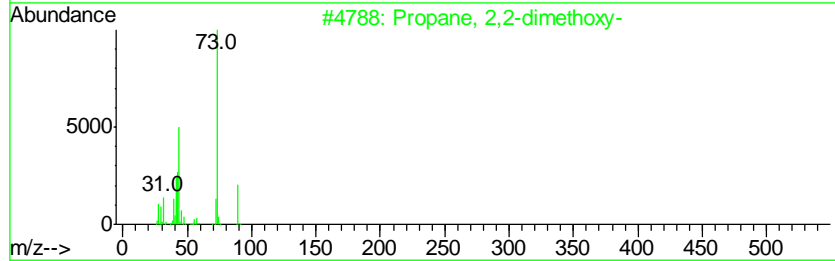
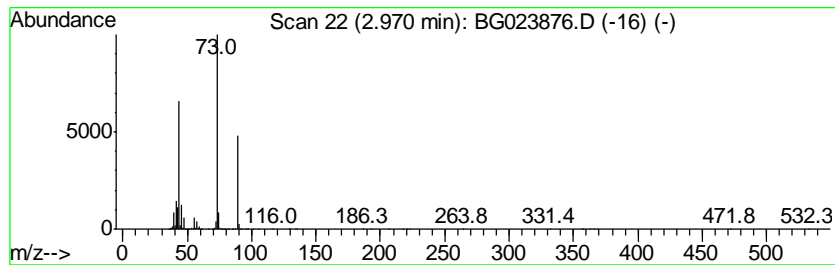
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 1 unknown2.97 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.97	293.38 ng	11867500	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4		1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	9
5		1-Propanol, 2-methyl-2-nitro-	119	C4H9NO3	000076-39-1	9



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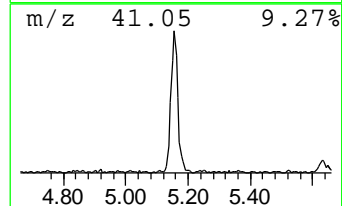
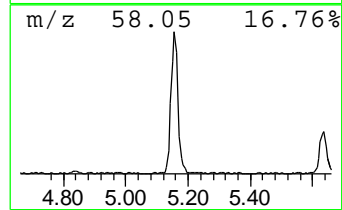
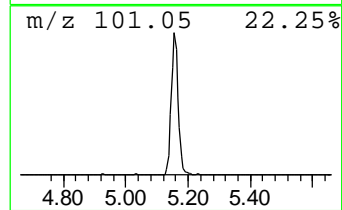
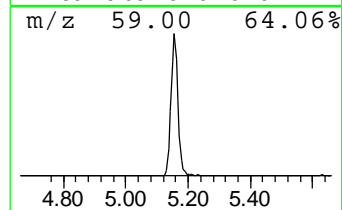
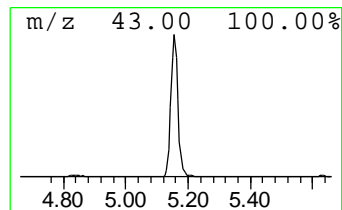
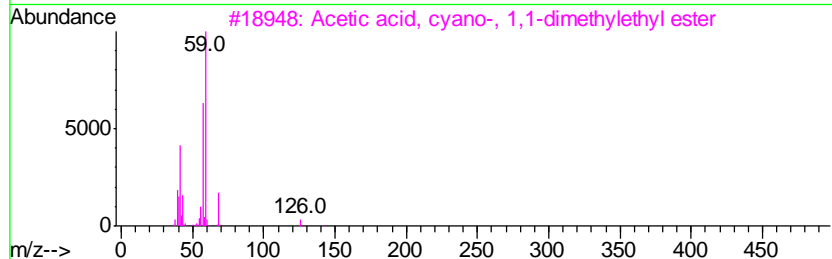
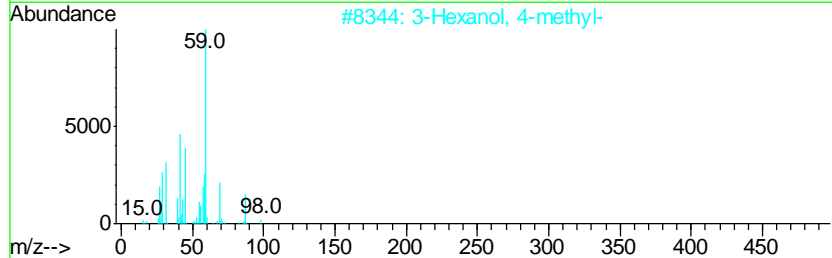
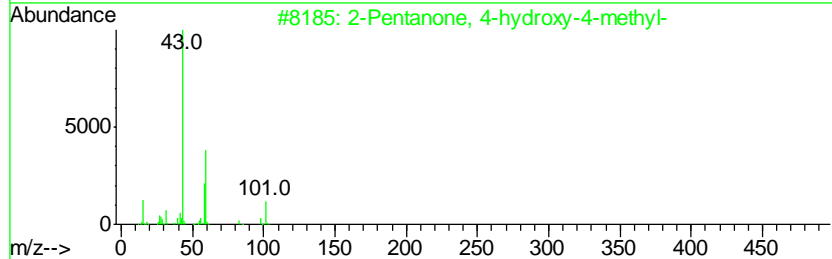
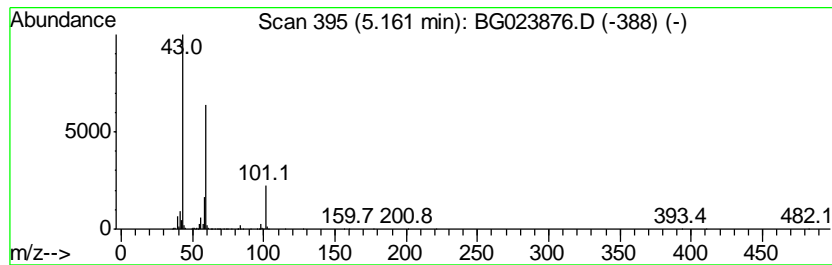
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 Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	29.64 ng	1199080	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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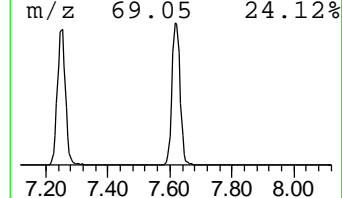
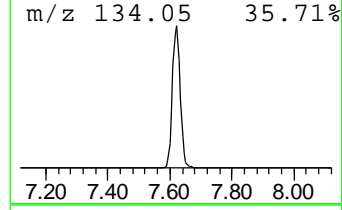
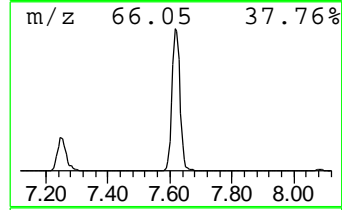
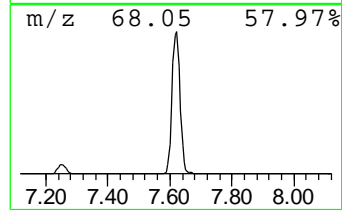
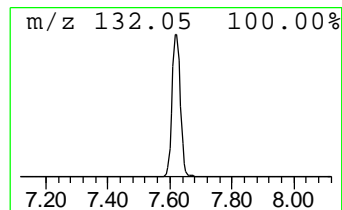
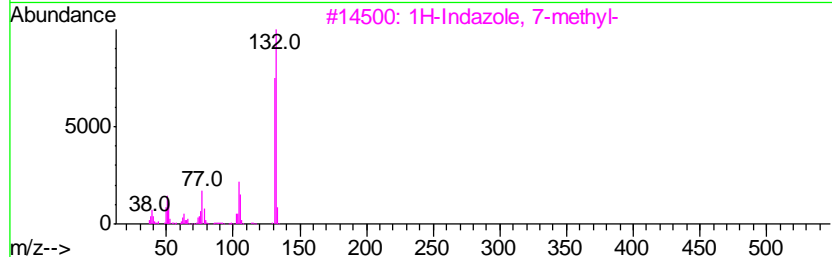
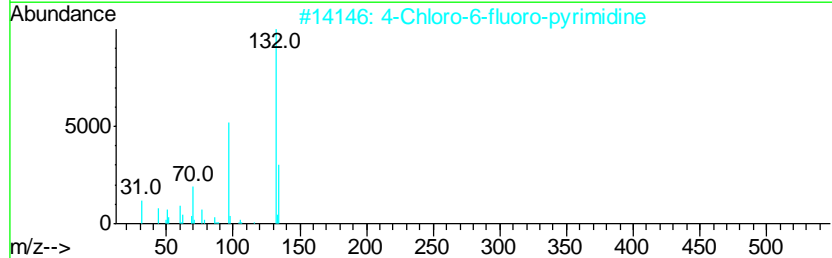
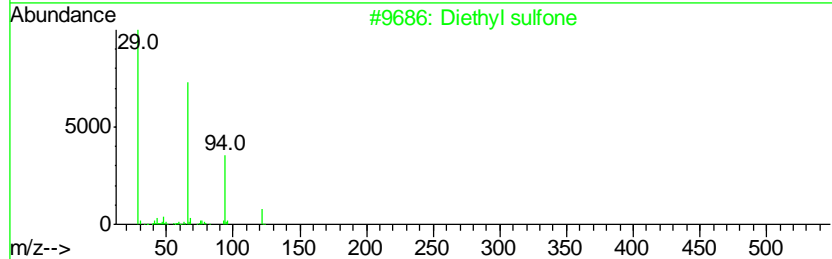
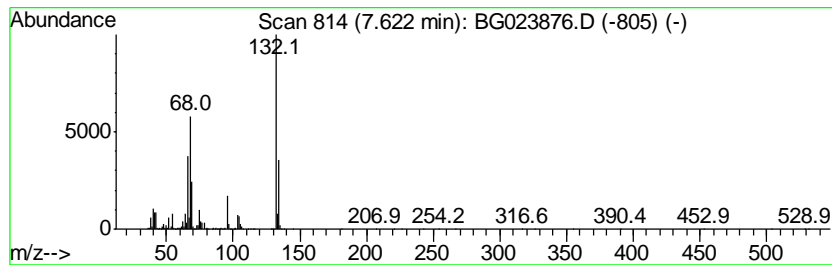
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 3 unknown7.62 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	93.96 ng	3800640	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethyl sulfone	122	C4H10O2S	000597-35-3	23
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



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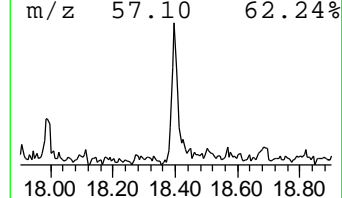
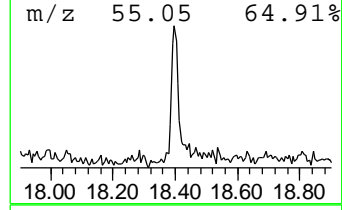
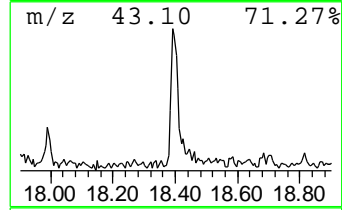
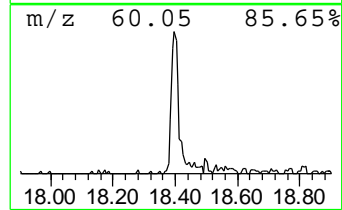
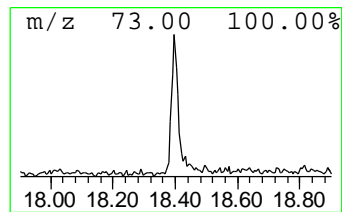
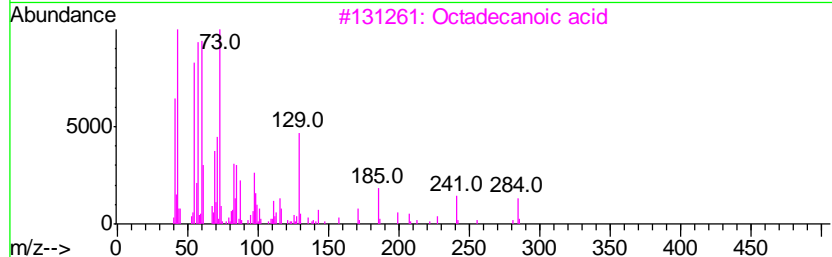
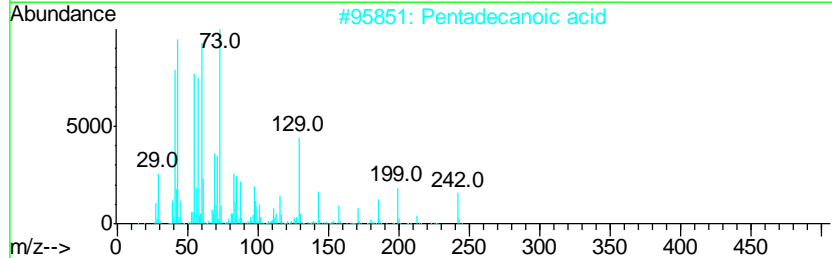
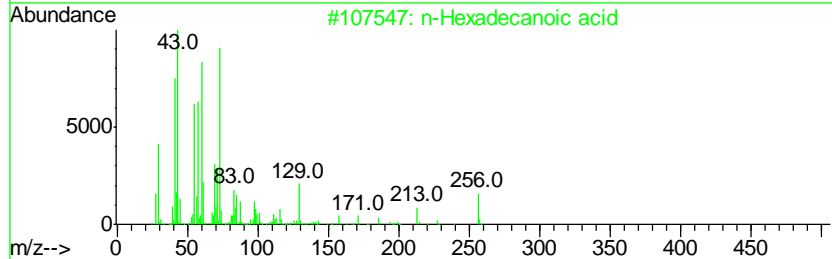
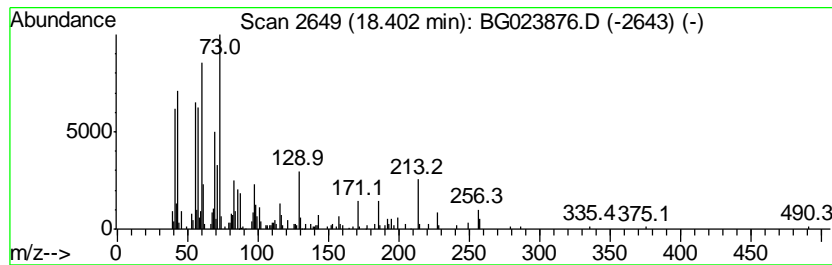
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TIC Library : C:\DATABASE\NIST11.L
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 Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.40	2.50 ng	245218	Phenanthrene-d10	17.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3		Octadecanoic acid	284	C18H36O2	000057-11-4	53
4		Tridecanoic acid	214	C13H26O2	000638-53-9	47
5		n-Decanoic acid	172	C10H20O2	000334-48-5	47



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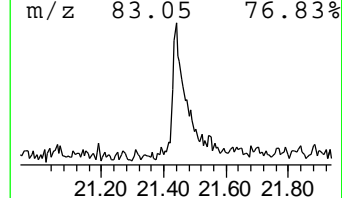
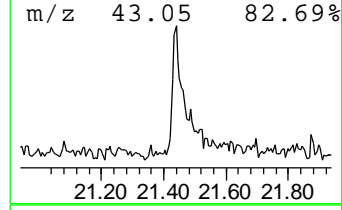
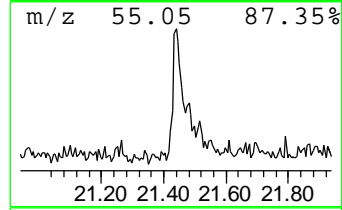
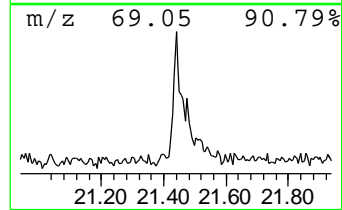
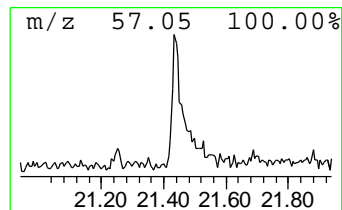
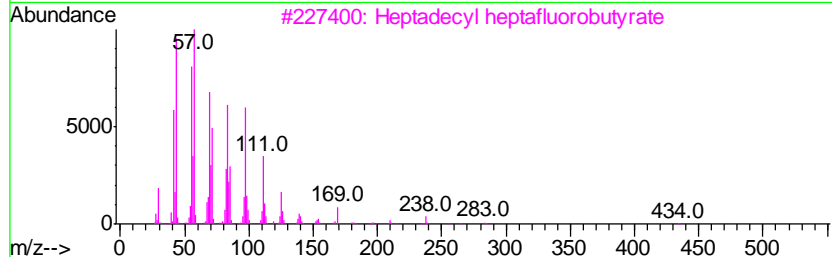
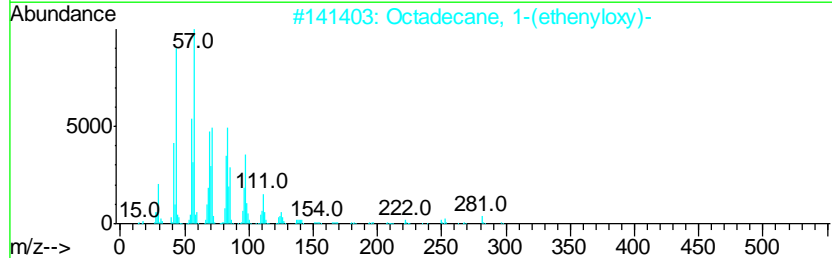
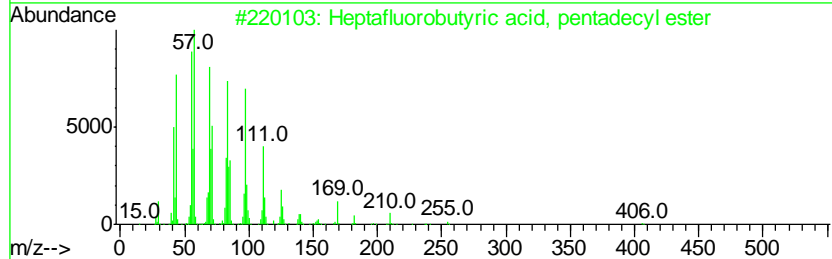
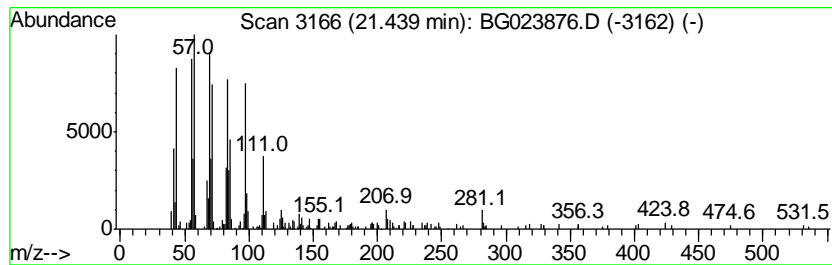
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TIC Library : C:\DATABASE\NIST11.L
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 Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.44	2.47 ng	282651	Chrysene-d12	21.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	81
2		Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	78
3		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	68
4		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	68
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	60



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.97	2.97	293.4	ng	11867500	1	8.09	809010	20.0
2-Pentanone, 4-hy...	5.16	29.6	ng	1199080	1	8.09	809010	20.0
unknown7.62	7.62	94.0	ng	3800640	1	8.09	809010	20.0
n-Hexadecanoic acid	18.40	2.5	ng	245218	4	17.53	1962050	20.0
Heptafluorobutyri...	21.44	2.5	ng	282651	5	21.84	2288500	20.0